

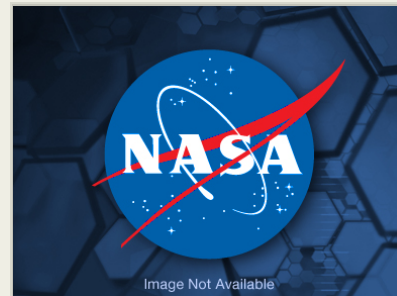
New Scan Modes in Ion Trap Mass Spectrometers for Planetary Exploration

Completed Technology Project (2016 - 2019)



Project Introduction

I. Objectives We propose modifications to the operation of the quadrupole mass filter and the quadrupole ion trap. New modes will alter the operating pressure, increase signal/noise ratios, and allow new types of scans, (e.g. precursor scans) in single analyzers. The modifications will include Hadamard multiplexed detection to increase signal/noise ratios and secular frequency scans to record mass spectra as well as MS/MS scans. The experiments will be implemented on both commercial and lab-built miniature instruments. Ions will be generated from solutions and from solids using ambient ionization methods. **II. Methods and Technology** The proposed work seeks to implement significant changes in the way mass spectrometers are operated to better match requirements of planetary exploration. These requirements include (i) small, light instruments, (ii) tandem mass spectrometry, including product, precursor, and neutral loss scans, (iii) simplified electronics, (iv) higher pressure operation, (v) improved sample utilization, and (vi) wet and dry sample ionization. Secular frequency scans Current benchtop and miniature mass spectrometers will be adapted to perform secular frequency scans using ac frequency ramps. Supplemental ac signals will be scanned across ions' secular frequencies while keeping the trapping radio frequency (rf) signal constant. Careful control of the amplitude and frequency in the ac signal(s) should allow novel MS and MS/MS scans to be performed, including precursor scans not previously possible in single analyzer instruments. Other scans (e.g. multiple reaction monitoring) are also accessible. These experiments remove the demanding electronics needed for rf amplitude sweep in current instruments. Operation at higher pressures is also anticipated. Hadamard multiplex measurements Secular frequency scanning will enable multiplexed Hadamard 'masking' detection, increasing signal/noise via the Fellgett-Jacquinet advantage. This will be accomplished by simultaneously interrogating (exciting or ejecting) multiple ions using ac voltages of appropriate frequencies. The use of stored waveform inverse Fourier transform notches should further increase the capabilities of the proposed scans by masking certain values of the Mathieu parameter, q , allowing rapid acquisition of the entire 2D precursor-product ion space. Wet and dry ambient soft ionization Wet samples will be ionized via relay electrospray using a small charge pulse (e.g. a primary electrospray). When this charge is incident on an insulated capillary containing a sample in solution, efficient ionization of the analytes occurs. Plasma methods based on a new miniature desorption atmospheric pressure chemical ionization source will serve as dry ionization techniques for solids and surface films. **III. Perceived Impact of the Proposed Work** The proposed work will integrate novel scan techniques, including multiplexing, into current quadrupole mass filters and ion traps to increase performance. The incorporation of unique methods of ambient ionization will provide improved ionization for both wet and dry samples. Such a system will allow the detection, identification, and structural elucidation of trace organics on Mars, Titan, and other planetary satellites and meteorites with high signal/noise, all while simplifying electronics. The use of precursor ion scans



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Organizational Responsibility

Responsible Mission Directorate:

Science Mission Directorate (SMD)

Responsible Program:

Planetary Instrument Concepts for the Advancement of Solar System Observations

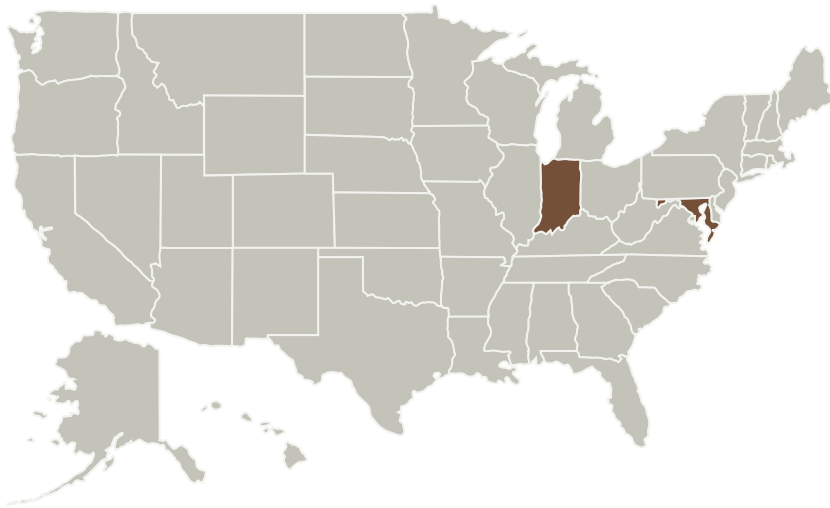
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will facilitate exploration for unknown organics. The experiments will also be performed using miniature systems that benefit from simple electronics and higher operating pressure. IV. Research and Development Team R. Graham Cooks, Distinguished Professor of Chemistry, Purdue University. Paul Mahaffy, Chief, Planetary Environment Laboratory, Solar System Exploration Division, NASA Goddard Space Flight Center

Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
Purdue University-Main Campus	Supporting Organization	Academia	West Lafayette, Indiana

Primary U.S. Work Locations	
Indiana	Maryland

Project Management

Program Director:

Carolyn R Mercer

Program Manager:

Haris Riris

Principal Investigator:

Robert G Cooks

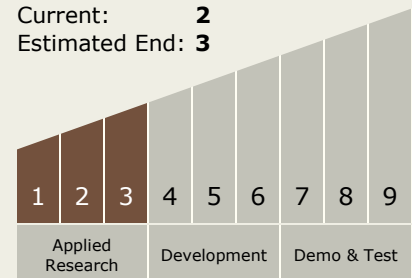
Co-Investigators:

Paul Mahaffy

Michael R Ludwig

Technology Maturity (TRL)

Start: 1
Current: 2
Estimated End: 3



Technology Areas

Primary:

- TX08 Sensors and Instruments
 - TX08.3 In-Situ Instruments and Sensors
 - TX08.3.4 Environment Sensors

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Target Destination

Others Inside the Solar System